

## REPORT DOCUMENTATION PAGE

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Final Tech Report, 01 Sep 93 - 31 May 97

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Modeling and Visualization for Polymers, Surfaces and Biomolecules

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F49620-93-1-0553

6. AUTHOR(S)

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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

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13. ABSTRACT (Maximum 200 words)

Problems in the representation of molecular surfaces using different spline representations have been studied. The suitability of these patch representations for visualizing scalar functions has been analyzed.

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Final Technical Progress Report  
(01 September 96 - 31 May 97)

Project Title: Modeling and Visualization for Polymers, Surfaces  
and Biomolecules

PI Name (Last, First, MI): \_\_Bajaj, Chandrajit, L.\_\_

Institution: \_\_Purdue University\_\_ 2304/DS

Contract/Grant No. \_\_ NM

Supplement) F49620-93-1-0553 (Aasert) NX NM (AASERT

Program Manager: Dr. Neal Glassman

SUMMARY OF RESEARCH OBJECTIVES

Our research emphasizes efficient algorithms and data structures for  
or  
biomolecular modeling and visualization.

The main research thrusts of this contract are:

1. The computation of the topological, combinatorial and metric properties of the molecular structure of polymers and biomolecules based on weighted  $\alpha$  shapes
2. The determination of similarities between two or more polymers or biomolecules based on geometric matching of the determined structural properties of the molecules
3. The development and graphical simulation of localized molecular docking strategies based on road map calculations on convolution surfaces of the interacting molecule structures and localized regions of the potential energy surfaces
4. The modeling, visualization and manipulation of the molecules together with their potential energy surfaces.
5. The implementation of the above algorithms in an existing distributed

(multi-user and multi-workstation)  
geometric software environment.

#### SUMMARY OF TECHNICAL PROGRESS

1. In our quest for real-time, interactive modeling and visualization of polymers, biomolecules, and associated scalar fields we have developed and implemented scattered data fitting algorithms in our SHASTRA distributed and collaborative software environment

The implementation is fully distributed, harnessing the collective power of networked workstations. It is capable of automatically reconstructing (accurately and smoothly) the union of balls structures as well as scalar fields such as electron density and potential energy surfaces.

This research is reported in publications 1, 2, 4, 5 and 6 below.

2. The AASERT supplement to the grant supported graduate students Susan Evans and

Dan Schikore. Together with Susan and Dan we studied problems in molecular surfaces (arbitrary topology) using different spline representations. Furthermore we analyze the suitability of these patch representations for visualizing scalar functions such as molecular orbitals and potential interaction energies.

This research has resulted in publications 3, 7, 8 below.

12. a. Number of AFOSR supported:

i. Papers published or accepted for publication in refereed journals: 1

ii. Papers published or accepted for publication in refereed conferences: 4

iii. Books or book chapters published or in press:

\_3

b. Trainee Data: Total 8 Female 2 Male 6

Minority 0 Non Us Citizen 5

- i. No. of Grad Students 6
- ii. No. of Postdoctorals 0
- iii. No. of Undergraduates 1

d. Awards/Honors to PI and/or members of PI's research group (please describe).

Awarded Visualization Chair, The University of Texas at Austin, Austin, TX.

Appointed Director of the Visualization Research Center with the Texas Institute of Computational and Applied Mathematics (TICAM), The University of Texas at Austin.

e. Brief description of all transitions (or intended transitions) of your ideas or techniques to industry, to military laboratories or to military application.

We have been collaborating with WPAFB, (Ruth Pachter) on our molecular modeling, docking and similarity computations. We provided our alpha shapes modeling and visualization software to Ruth and her group to enable them to visualize molecular surfaces and properties (using our A-splines) for siloxane polymers with NLO moieties. This visualization shall be coupled to the GROPE system which WPAFB has recently acquired.

Adittionally, we plan to transition Dynamic Mesh Simplification, Compression and Visualization Techniques to the Institute of Defense Analysis,

Arlington, VA.

g. Attach list of papers and other publications with full citation.

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[1] ``Rational Parameterizations of Nonsingular Cubic Surfaces'', (with R. Holt and A. Netravali).

Full version accepted for publication in {ACM Transactions on Graphics}, (1997).

[2] Book: {\sf Scientific Visualization Techniques}, John Wiley and Sons, (1997)

[3] ``Splines and Geometric Modeling'', (with S. Evans)  
{CRC Handbook of Discrete and Computational Geometry},  
edited by J. Goodman and J. O'Rourke,  
CRC Series, {Discrete and Combinatorial Mathematics},  
(1997), 833 - 849.

[4] Book Chapter: ``Implicit Surface Patches'',  
{Introduction to Implicit Surfaces}, edited by J. Bloomenthal,  
{Morgan Kaufman Publishers}, (1997), 98 - 125.

[5] ``Interrogative Data Visualization'',  
(Invited Paper at the 7th IMA Conference on the Mathematics of Surfaces),  
{The Mathematics of Surfaces VII},  
edited by T.N.T. Goodman and R. Martin, {Oxford University Press},  
(1997).

[6] ``NURBS based B-rep Models for Macromolecules and their Properties'',  
(with H-Y. Lee, R. Merkert, V. Pascucci),  
{Proc. of the 1997 ACM Symposium on Solid Modeling},  
ACM Press, (1997), Atlanta, Georgia, 217 - 228.

[7] ``Contour Trees and Small Seed Sets for Isosurface Traversal''  
,  
(with M. van Kreveld, R. van Oostrum, V. Pascucci, D.  
Schikore)  
{Proc. of the 13th Annual ACM Symposium on Computational  
Geometry},  
ACM Press, (1997), Nice, France, 212 - 219.

[8] ``The Contour Spectrum'',  
(with V. Pascucci, D. Schikore)  
{Proc. of the Annual IEEE Visualization Conference},  
IEEE Computer Society Press, (1997), Phoenix, Arizona.

#### h. List of Invited Presentations

Dagstuhl-Seminar on Scientific Visualization, Schloss Dagstuhl,  
West Germany, May 1997.

Minisymposium on Reverse Engineering,  
Conference on Computer Aided Geometric Design, Lillehammer, Norw  
ay,  
July 1997.

IMACS conference on Problem Solving Environments  
Berlin, Germany, August 1997.

Invited Speaker at the Laredo Course on Applications of Symbolic  
Computing, Laredo, Spain, September 1997.

Invited Speaker for a Tutorial at Eurographics '97, Budapest,  
Hungary, September 1997.

Invited Speaker for the Conference on New Themes in Computer Aide  
d  
Geometric Modeling, Tel-Aviv, Israel, February 1998

Invited Speaker at the Mathematisches Forschungsinstitut  
Oberwolfach Seminar on Free-Form Curves and Surfaces, West Germa  
ny,  
June 1998.

i. List of Program Committees Served

Pacific Graphics '97, Korea, 1997

Computer Graphics International '97, Belgium, 1997.

Workshop on Algorithms and Data Structures '97, WADS, Halifax, Canada 1997.

Program Committee Member of the IEEE Visualization Conference '97, Phoenix, Arizona, October 1997.

Program Committee Member of Fifth International Conference on Computer-Aided Design and Computer Graphics, Shenzhen, China, December 1997.

Program Committee Member of the ACM symposium on Computational Geometry (Theory) Minneapolis, MN, June 1998.

Program Committee Member of IMA Math of Surfaces VIII, Birmingham, UK, August 1998.